



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 1ULT / pdb_00001ult
Title : Crystal structure of tt0168 from *Thermus thermophilus* HB8
Authors : Hisanaga, Y.; Ago, H.; Nakatsu, T.; Hamada, K.; Ida, K.; Kanda, H.; Yamamoto, M.; Hori, T.; Arii, Y.; Sugahara, M.; Kuramitsu, S.; Yokoyama, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-09-16
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

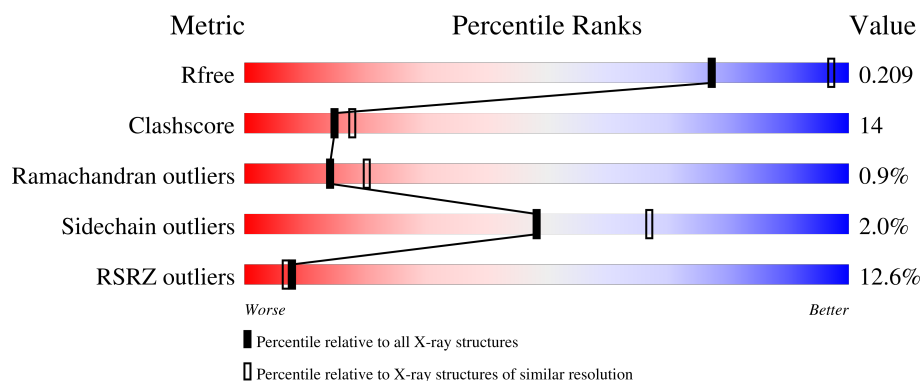
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	541	6% 69% 28% ..
1	B	541	18% 69% 24% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	1001	-	X	-	-

2 Entry composition [i](#)

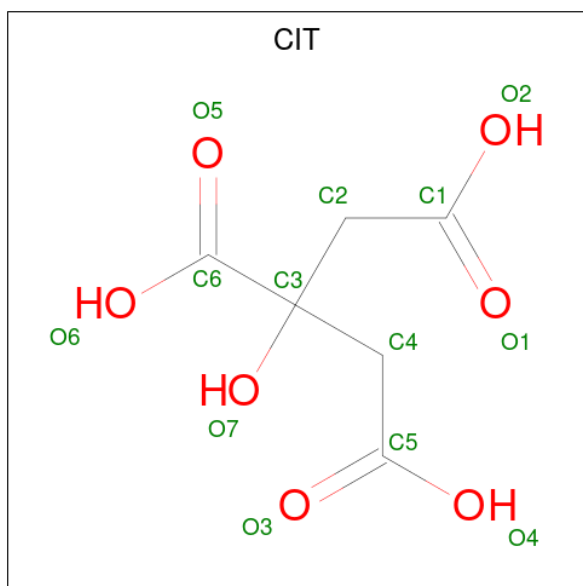
There are 3 unique types of molecules in this entry. The entry contains 8431 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called long chain fatty acid-CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4142	2653	721	757	11			
1	B	514	Total	C	N	O	S	0	0	0
			3989	2551	693	734	11			

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		

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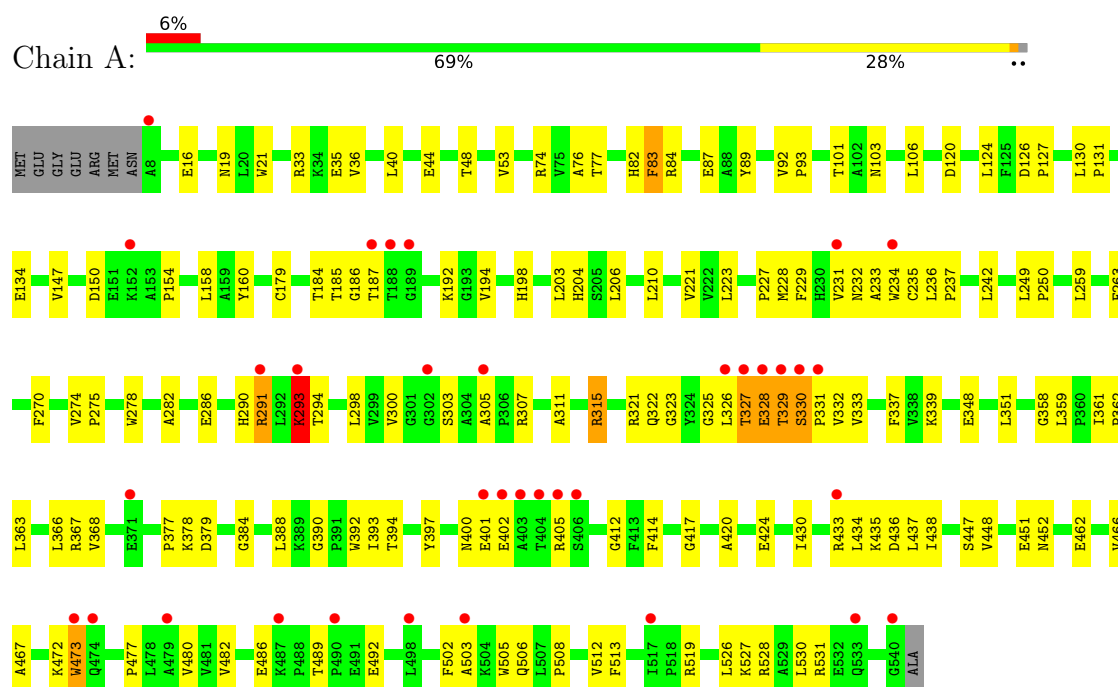
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	134	Total 134	O 134	0	0

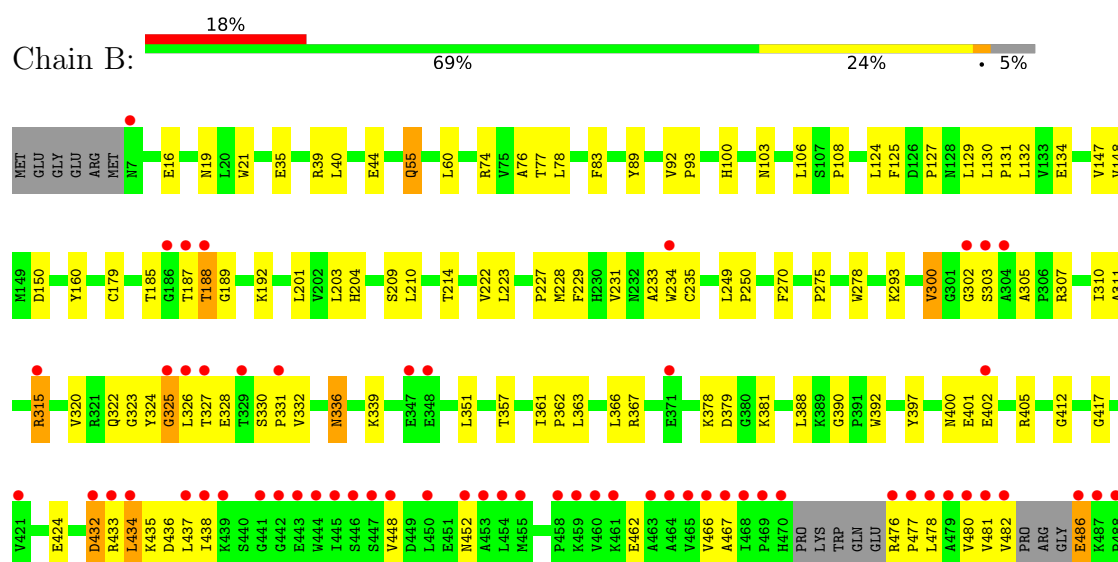
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: long chain fatty acid-CoA ligase



- Molecule 1: long chain fatty acid-CoA ligase



T489	P490	E491	E492	L493	M494	E495	H496	L497	L498	K499	A500	G501	PHE	ALA	LYS	TRP	GLN	LEU	PRO	D509	A510	Y511	V512	F513	A514	E515	E516	T517	P518	R519	T520	SER	ALA	GLY	LYS	F525	L526	K527	R528	A529	L530	R531	E532	Q533	Y534	K535	N536	Y537	Y538	G539	GLY	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.95Å 124.69Å 212.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.55 49.64 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.64-2.55) 97.4 (49.64-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.51 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.239 0.208 , 0.209	Depositor DCC
R_{free} test set	2446 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/4242	0.91	19/5765 (0.3%)
1	B	0.40	0/4077	0.89	13/5535 (0.2%)
All	All	0.40	0/8319	0.90	32/11300 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	THR	N-CA-C	-7.06	103.77	112.38
1	B	249	LEU	CA-C-N	6.99	127.14	119.87
1	B	249	LEU	C-N-CA	6.99	127.14	119.87
1	B	293	LYS	N-CA-C	6.82	118.72	111.28
1	A	330	SER	N-CA-C	6.66	120.03	109.64
1	A	249	LEU	CA-C-N	6.50	126.12	119.56
1	A	249	LEU	C-N-CA	6.50	126.12	119.56
1	A	482	VAL	N-CA-C	-6.44	101.78	108.15
1	A	388	LEU	N-CA-C	6.13	119.02	109.52
1	A	390	GLY	CA-C-N	6.11	126.56	119.47
1	A	390	GLY	C-N-CA	6.11	126.56	119.47
1	B	388	LEU	N-CA-C	5.93	118.72	109.52
1	A	83	PHE	N-CA-C	5.87	119.26	111.75
1	B	35	GLU	N-CA-C	5.67	118.87	110.48
1	B	83	PHE	N-CA-C	5.67	118.18	111.33
1	A	293	LYS	N-CA-C	5.54	117.76	111.11
1	A	35	GLU	N-CA-C	5.54	118.68	110.48
1	B	222	VAL	N-CA-C	5.54	116.28	108.36
1	A	250	PRO	N-CA-C	5.49	120.72	113.86
1	B	250	PRO	N-CA-C	5.45	120.73	114.03
1	A	358	GLY	N-CA-C	5.41	117.73	110.43
1	B	417	GLY	N-CA-C	-5.34	107.90	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	VAL	CA-C-N	5.34	125.33	119.89
1	A	482	VAL	C-N-CA	5.34	125.33	119.89
1	A	221	VAL	N-CA-C	-5.29	98.36	107.24
1	B	412	GLY	N-CA-C	5.22	122.79	115.43
1	A	417	GLY	N-CA-C	-5.22	108.12	115.32
1	A	412	GLY	N-CA-C	5.13	122.67	115.43
1	A	294	THR	N-CA-C	5.10	119.56	113.23
1	B	179	CYS	N-CA-C	-5.06	108.13	114.56
1	B	390	GLY	CA-C-N	5.04	124.83	119.28
1	B	390	GLY	C-N-CA	5.04	124.83	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4142	0	4165	125	0
1	B	3989	0	4008	104	0
2	A	13	0	5	3	0
3	A	153	0	0	5	0
3	B	134	0	0	1	0
All	All	8431	0	8178	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:CG2	1:A:394:THR:HG22	1.89	1.02
1:A:329:THR:HG22	1:A:394:THR:HG22	1.42	0.97
1:A:330:SER:HB3	1:A:393:ILE:HD13	1.61	0.82
1:B:92:VAL:HB	1:B:93:PRO:HD3	1.67	0.77
1:B:315:ARG:HG3	1:B:315:ARG:HH11	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLY:HA2	1:B:330:SER:O	1.85	0.76
1:A:311:ALA:HB1	1:A:315:ARG:HH12	1.53	0.73
1:A:329:THR:HG23	1:A:394:THR:HG22	1.69	0.73
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.72	0.71
1:B:231:VAL:HG21	1:B:326:LEU:HA	1.73	0.70
1:B:438:ILE:HD13	1:B:477:PRO:HB3	1.75	0.69
1:A:435:LYS:NZ	2:A:1001:CIT:H42	2.09	0.67
1:A:329:THR:HG22	1:A:394:THR:CG2	2.24	0.66
1:A:433:ARG:HG3	1:A:434:LEU:HD13	1.76	0.66
1:B:432:ASP:HA	1:B:448:VAL:HG21	1.76	0.66
1:A:477:PRO:HG2	1:A:508:PRO:HA	1.78	0.66
1:B:401:GLU:O	1:B:405:ARG:HG3	1.95	0.65
1:A:307:ARG:NH1	1:A:351:LEU:HD23	2.11	0.65
1:A:210:LEU:HD23	1:B:210:LEU:HD23	1.77	0.65
1:B:432:ASP:OD1	1:B:448:VAL:HG23	1.97	0.65
1:B:275:PRO:HG2	1:B:303:SER:HB2	1.79	0.65
1:A:194:VAL:HG21	1:A:328:GLU:HA	1.80	0.64
1:B:489:THR:OG1	1:B:492:GLU:HG3	1.98	0.64
1:A:400:ASN:HD22	1:A:400:ASN:C	2.03	0.64
1:A:435:LYS:HD3	2:A:1001:CIT:H22	1.78	0.64
1:A:435:LYS:HZ1	2:A:1001:CIT:H42	1.64	0.63
1:B:400:ASN:C	1:B:400:ASN:HD22	2.06	0.63
1:A:402:GLU:HG2	1:A:405:ARG:NH2	2.14	0.62
1:B:307:ARG:NH1	1:B:351:LEU:HD23	2.13	0.62
1:B:325:GLY:HA3	1:B:331:PRO:O	1.98	0.62
1:A:329:THR:HG21	1:A:414:PHE:CD2	2.34	0.62
1:A:234:TRP:HH2	1:A:323:GLY:HA3	1.64	0.62
1:A:311:ALA:HB1	1:A:315:ARG:NH1	2.15	0.61
1:A:438:ILE:HD13	1:A:477:PRO:HB3	1.83	0.61
1:A:231:VAL:CG1	1:A:327:THR:HA	2.30	0.61
1:B:536:ASN:OD1	1:B:539:GLY:HA2	2.00	0.60
1:A:489:THR:OG1	1:A:492:GLU:HG3	2.02	0.60
1:B:327:THR:HG23	1:B:330:SER:H	1.65	0.60
1:B:476:ARG:CZ	1:B:476:ARG:HA	2.31	0.60
1:A:275:PRO:HG2	1:A:303:SER:HB2	1.83	0.59
1:A:401:GLU:O	1:A:405:ARG:HG3	2.02	0.59
1:A:326:LEU:HD12	1:A:326:LEU:N	2.18	0.59
1:B:231:VAL:HG12	1:B:231:VAL:O	2.01	0.59
1:A:433:ARG:HG3	1:A:434:LEU:CD1	2.32	0.58
1:A:84:ARG:HD3	1:A:160:TYR:CD1	2.38	0.58
1:B:462:GLU:CD	1:B:519:ARG:HH22	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:C	1:A:223:LEU:HD23	2.29	0.57
1:B:512:VAL:HG12	1:B:513:PHE:N	2.19	0.57
1:A:329:THR:HG22	1:A:394:THR:N	2.19	0.57
1:B:223:LEU:HD23	1:B:223:LEU:C	2.30	0.57
1:A:420:ALA:HB2	1:A:430:ILE:HA	1.87	0.57
1:A:433:ARG:HA	1:A:437:LEU:HD12	1.87	0.57
1:A:311:ALA:O	1:A:315:ARG:HG3	2.05	0.56
1:B:366:LEU:C	1:B:366:LEU:HD23	2.31	0.56
1:A:329:THR:HG21	1:A:414:PHE:CG	2.41	0.56
1:A:325:GLY:HA3	1:A:331:PRO:O	2.06	0.55
1:B:315:ARG:HG3	1:B:315:ARG:NH1	2.21	0.55
1:B:366:LEU:HD23	1:B:367:ARG:N	2.21	0.55
1:A:203:LEU:HD21	1:B:203:LEU:HD21	1.87	0.54
1:A:321:ARG:HD3	3:A:1064:HOH:O	2.08	0.54
1:A:83:PHE:CZ	1:A:84:ARG:NH1	2.75	0.54
1:B:234:TRP:HH2	1:B:323:GLY:HA3	1.73	0.54
1:B:201:LEU:HD13	3:B:615:HOH:O	2.08	0.54
1:A:19:ASN:HD22	1:A:21:TRP:H	1.55	0.53
1:A:103:ASN:HB3	1:A:106:LEU:HG	1.90	0.53
1:A:462:GLU:CD	1:A:519:ARG:HH22	2.15	0.53
1:B:39:ARG:HG3	1:B:39:ARG:HH11	1.73	0.53
1:B:233:ALA:O	1:B:234:TRP:HB2	2.07	0.53
1:A:305:ALA:H	1:A:322:GLN:HE21	1.57	0.53
1:A:466:VAL:HG12	1:A:527:LYS:HD3	1.90	0.53
1:A:526:LEU:CD2	1:A:528:ARG:HB3	2.38	0.53
1:A:512:VAL:HG12	1:A:513:PHE:N	2.24	0.52
1:A:234:TRP:CH2	1:A:323:GLY:HA3	2.41	0.52
1:B:527:LYS:O	1:B:531:ARG:HG3	2.10	0.52
1:A:40:LEU:HD12	1:A:44:GLU:CG	2.39	0.52
1:B:204:HIS:NE2	1:B:332:VAL:HB	2.24	0.52
1:B:476:ARG:HA	1:B:476:ARG:NE	2.25	0.52
1:A:74:ARG:HD3	1:A:74:ARG:N	2.25	0.51
1:A:526:LEU:HD23	1:A:528:ARG:HB3	1.92	0.51
1:A:124:LEU:HD23	1:A:147:VAL:HB	1.93	0.51
1:B:378:LYS:HB2	1:B:424:GLU:OE2	2.09	0.51
1:B:432:ASP:HA	1:B:448:VAL:CG2	2.39	0.51
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.45	0.51
1:B:526:LEU:HD23	1:B:528:ARG:HB3	1.93	0.51
1:A:366:LEU:C	1:A:366:LEU:HD23	2.35	0.51
1:A:473:TRP:H	1:A:473:TRP:CD1	2.26	0.51
1:A:329:THR:HA	1:A:394:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:PHE:HA	1:A:506:GLN:NE2	2.26	0.51
1:B:311:ALA:O	1:B:315:ARG:HG3	2.10	0.50
1:A:19:ASN:ND2	1:A:21:TRP:H	2.08	0.50
1:A:329:THR:HG22	1:A:394:THR:H	1.75	0.50
1:A:480:VAL:HG21	1:A:530:LEU:HD22	1.93	0.50
1:A:330:SER:CB	1:A:333:VAL:HG13	2.41	0.50
1:B:209:SER:HA	1:B:214:THR:OG1	2.11	0.50
1:A:278:TRP:HA	1:A:278:TRP:HE3	1.75	0.50
1:A:361:ILE:HD11	1:A:392:TRP:CZ2	2.46	0.50
1:B:278:TRP:HA	1:B:278:TRP:CE3	2.47	0.50
1:B:438:ILE:HG12	1:B:467:ALA:HB2	1.94	0.50
1:B:509:ASP:O	1:B:510:ALA:HB2	2.12	0.50
1:B:311:ALA:C	1:B:315:ARG:NH1	2.69	0.50
1:B:60:LEU:HD22	1:B:160:TYR:OH	2.11	0.49
1:B:103:ASN:HB3	1:B:106:LEU:HG	1.94	0.49
1:A:531:ARG:HD2	3:A:1134:HOH:O	2.11	0.49
1:B:187:THR:O	1:B:189:GLY:N	2.46	0.49
1:A:76:ALA:HB2	1:A:120:ASP:OD2	2.13	0.49
1:A:400:ASN:C	1:A:400:ASN:ND2	2.71	0.49
1:B:336:ASN:C	1:B:336:ASN:HD22	2.20	0.49
1:A:101:THR:HB	1:A:229:PHE:HA	1.95	0.49
1:A:433:ARG:HA	1:A:437:LEU:HB2	1.95	0.49
1:A:330:SER:HB2	1:A:333:VAL:HG13	1.94	0.48
1:B:325:GLY:CA	1:B:330:SER:O	2.56	0.48
1:B:526:LEU:CD2	1:B:528:ARG:HB3	2.43	0.48
1:B:436:ASP:HA	1:B:531:ARG:HH21	1.78	0.48
1:B:234:TRP:O	1:B:235:CYS:HB2	2.12	0.48
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.96	0.48
1:B:234:TRP:CH2	1:B:323:GLY:HA3	2.49	0.48
1:B:402:GLU:HG2	1:B:405:ARG:NH2	2.29	0.48
1:A:298:LEU:C	1:A:298:LEU:HD23	2.39	0.47
1:A:33:ARG:HD2	3:A:1078:HOH:O	2.14	0.47
1:A:124:LEU:CD2	1:A:147:VAL:HB	2.45	0.47
1:A:377:PRO:HB2	1:A:379:ASP:OD2	2.14	0.47
1:A:527:LYS:O	1:A:531:ARG:HG3	2.14	0.47
1:B:278:TRP:HA	1:B:278:TRP:HE3	1.78	0.47
1:A:378:LYS:HB2	1:A:424:GLU:OE2	2.14	0.47
1:B:124:LEU:CD2	1:B:147:VAL:HB	2.44	0.47
1:B:270:PHE:CD1	1:B:270:PHE:C	2.93	0.47
1:B:74:ARG:HD3	1:B:74:ARG:N	2.30	0.47
1:A:361:ILE:HD11	1:A:392:TRP:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:VAL:HG12	1:B:527:LYS:HD3	1.97	0.47
1:B:40:LEU:HD12	1:B:44:GLU:CG	2.45	0.47
1:B:227:PRO:HB3	1:B:229:PHE:CE2	2.50	0.47
1:A:82:HIS:HE1	1:A:126:ASP:OD1	1.98	0.46
1:B:305:ALA:H	1:B:322:GLN:HE21	1.62	0.46
1:B:311:ALA:CB	1:B:315:ARG:HH12	2.28	0.46
1:B:400:ASN:C	1:B:400:ASN:ND2	2.71	0.46
1:A:228:MET:HA	1:A:233:ALA:HB2	1.97	0.46
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.30	0.46
1:A:438:ILE:CD1	1:A:477:PRO:HB3	2.45	0.46
1:A:242:LEU:HD11	1:B:362:PRO:HB3	1.97	0.46
1:A:274:VAL:HG22	3:A:1093:HOH:O	2.15	0.46
1:A:366:LEU:HD23	1:A:367:ARG:N	2.31	0.46
1:B:325:GLY:HA3	1:B:331:PRO:C	2.40	0.46
1:B:478:LEU:HD11	1:B:512:VAL:HG23	1.96	0.46
1:B:435:LYS:C	1:B:437:LEU:H	2.23	0.46
1:A:290:HIS:O	1:A:291:ARG:HD3	2.16	0.46
1:A:77:THR:HA	1:A:124:LEU:O	2.16	0.45
1:A:89:TYR:OH	1:A:232:ASN:HA	2.16	0.45
1:B:19:ASN:ND2	1:B:21:TRP:H	2.15	0.45
1:B:192:LYS:HB3	1:B:397:TYR:CD1	2.50	0.45
1:A:53:VAL:HG13	1:A:87:GLU:HG2	1.98	0.45
1:B:494:ASN:O	1:B:498:LEU:HG	2.17	0.45
1:A:447:SER:O	1:A:451:GLU:HG2	2.16	0.45
1:B:311:ALA:HB1	1:B:315:ARG:HH12	1.82	0.45
1:B:481:VAL:HG12	1:B:482:VAL:N	2.32	0.45
1:B:438:ILE:CD1	1:B:477:PRO:HB3	2.46	0.45
1:B:328:GLU:CD	1:B:328:GLU:H	2.25	0.45
1:A:179:CYS:HB3	1:A:198:HIS:CD2	2.52	0.44
1:B:108:PRO:HG3	1:B:132:LEU:CD1	2.47	0.44
1:B:324:TYR:HB2	1:B:357:THR:CG2	2.48	0.44
1:A:127:PRO:HG3	1:A:150:ASP:HB2	1.99	0.44
1:A:330:SER:HB3	1:A:393:ILE:CD1	2.41	0.44
1:A:282:ALA:O	1:A:286:GLU:HG3	2.17	0.44
1:A:76:ALA:HB2	1:A:120:ASP:CG	2.42	0.44
1:A:330:SER:CB	1:A:333:VAL:CG1	2.96	0.44
1:A:503:ALA:HB3	1:A:505:TRP:CD1	2.53	0.44
1:B:512:VAL:CG1	1:B:513:PHE:N	2.81	0.44
1:A:185:THR:C	1:A:187:THR:H	2.26	0.43
1:A:274:VAL:HG13	3:A:1093:HOH:O	2.18	0.43
1:A:147:VAL:HA	1:A:158:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PRO:HG3	1:B:150:ASP:HB2	2.00	0.43
1:A:305:ALA:H	1:A:322:GLN:NE2	2.16	0.43
1:B:55:GLN:HE21	1:B:55:GLN:HB3	1.68	0.43
1:A:130:LEU:HD21	1:A:154:PRO:HG2	1.99	0.43
1:B:125:PHE:CZ	1:B:148:VAL:HG22	2.53	0.43
1:B:361:ILE:HD11	1:B:392:TRP:CZ2	2.54	0.43
1:B:361:ILE:HD11	1:B:392:TRP:HZ2	1.84	0.43
1:B:379:ASP:OD1	1:B:381:LYS:N	2.45	0.43
1:A:184:THR:HG21	1:A:328:GLU:OE2	2.18	0.43
1:B:76:ALA:HA	1:B:100:HIS:O	2.19	0.43
1:B:448:VAL:HG12	1:B:452:ASN:ND2	2.33	0.43
1:A:448:VAL:HG12	1:A:452:ASN:ND2	2.34	0.43
1:B:302:GLY:HA3	1:B:326:LEU:HD23	2.01	0.42
1:B:310:ILE:HG23	1:B:320:VAL:HB	2.00	0.42
1:B:490:PRO:O	1:B:494:ASN:ND2	2.53	0.42
1:B:19:ASN:ND2	1:B:21:TRP:HB3	2.34	0.42
1:A:36:VAL:HB	1:A:48:THR:HG23	2.02	0.42
1:A:307:ARG:NH2	1:A:348:GLU:O	2.52	0.42
1:B:77:THR:HA	1:B:124:LEU:O	2.19	0.42
1:B:187:THR:O	1:B:188:THR:C	2.63	0.42
1:B:476:ARG:HG2	1:B:476:ARG:HH11	1.84	0.42
1:A:83:PHE:O	1:A:87:GLU:HG3	2.19	0.42
1:A:326:LEU:C	1:A:328:GLU:N	2.74	0.42
1:A:486:GLU:O	1:A:486:GLU:HG3	2.18	0.42
1:B:185:THR:C	1:B:187:THR:H	2.27	0.42
1:B:228:MET:HA	1:B:233:ALA:HB2	2.02	0.42
1:A:503:ALA:O	1:A:506:GLN:HG2	2.19	0.42
1:B:476:ARG:NH2	1:B:477:PRO:HD2	2.33	0.42
1:A:293:LYS:H	1:A:293:LYS:HD2	1.84	0.42
1:B:204:HIS:HD2	1:B:392:TRP:CE2	2.38	0.42
1:A:270:PHE:CD1	1:A:270:PHE:C	2.98	0.42
1:A:436:ASP:OD1	1:A:448:VAL:HG23	2.20	0.42
1:B:124:LEU:HD23	1:B:147:VAL:HB	2.01	0.41
1:A:259:LEU:HB3	1:A:263:PHE:CE2	2.55	0.41
1:A:368:VAL:HG12	1:A:384:GLY:HA3	2.02	0.41
1:A:502:PHE:HA	1:A:506:GLN:HE21	1.84	0.41
1:A:512:VAL:CG1	1:A:513:PHE:N	2.83	0.41
1:A:234:TRP:O	1:A:235:CYS:HB2	2.20	0.41
1:A:337:PHE:CE1	1:A:359:LEU:HD12	2.56	0.41
1:B:78:LEU:O	1:B:129:LEU:HD12	2.20	0.41
1:A:329:THR:CB	1:A:394:THR:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:O	1:B:434:LEU:C	2.64	0.41
1:B:486:GLU:OE1	1:B:486:GLU:N	2.53	0.41
1:B:519:ARG:HB3	1:B:520:THR:H	1.69	0.41
1:B:130:LEU:N	1:B:131:PRO:CD	2.84	0.41
1:A:192:LYS:HB3	1:A:397:TYR:CD1	2.56	0.40
1:A:236:LEU:HB2	1:A:237:PRO:HD3	2.02	0.40
1:A:227:PRO:HB3	1:A:229:PHE:CE2	2.57	0.40
1:A:438:ILE:HG12	1:A:467:ALA:HB2	2.04	0.40
1:B:300:VAL:HG21	1:B:305:ALA:HB2	2.03	0.40
1:A:206:LEU:HD11	1:B:363:LEU:HD11	2.03	0.40
1:A:330:SER:HA	1:A:331:PRO:HD3	1.94	0.40
1:A:362:PRO:O	1:A:363:LEU:HB2	2.20	0.40
1:B:480:VAL:HG21	1:B:530:LEU:HD22	2.03	0.40
1:A:84:ARG:HH21	1:A:150:ASP:HA	1.86	0.40
1:A:204:HIS:NE2	1:A:332:VAL:HB	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/541 (98%)	510 (96%)	17 (3%)	4 (1%)	16	22
1	B	504/541 (93%)	484 (96%)	15 (3%)	5 (1%)	12	17
All	All	1035/1082 (96%)	994 (96%)	32 (3%)	9 (1%)	14	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	THR
1	B	434	LEU
1	A	328	GLU

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Mol	Chain	Res	Type
1	A	329	THR
1	B	432	ASP
1	A	472	LYS
1	B	510	ALA
1	A	186	GLY
1	B	325	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/437 (99%)	423 (98%)	8 (2%)	50	69
1	B	417/437 (95%)	408 (98%)	9 (2%)	45	64
All	All	848/874 (97%)	831 (98%)	17 (2%)	48	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	134	GLU
1	A	291	ARG
1	A	293	LYS
1	A	300	VAL
1	A	315	ARG
1	A	339	LYS
1	A	473	TRP
1	B	16	GLU
1	B	55	GLN
1	B	89	TYR
1	B	134	GLU
1	B	300	VAL
1	B	315	ARG
1	B	336	ASN
1	B	339	LYS
1	B	486	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	55	GLN
1	A	82	HIS
1	A	128	ASN
1	A	144	GLN
1	A	290	HIS
1	A	322	GLN
1	A	335	GLN
1	A	400	ASN
1	A	452	ASN
1	A	474	GLN
1	A	494	ASN
1	A	506	GLN
1	B	19	ASN
1	B	55	GLN
1	B	128	ASN
1	B	144	GLN
1	B	290	HIS
1	B	322	GLN
1	B	335	GLN
1	B	336	ASN
1	B	400	ASN
1	B	452	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	1001	-	12,12,12	2.01	4 (33%)	17,17,17	2.98	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	1001	-	-	11/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CIT	C3-C6	4.00	1.57	1.53
2	A	1001	CIT	O7-C3	3.51	1.49	1.43
2	A	1001	CIT	O5-C6	2.47	1.29	1.22
2	A	1001	CIT	O1-C1	2.30	1.29	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	CIT	O7-C3-C6	-7.86	97.82	108.96
2	A	1001	CIT	O5-C6-C3	-4.34	113.68	122.09
2	A	1001	CIT	C2-C3-C6	3.60	117.99	110.03
2	A	1001	CIT	O2-C1-C2	3.40	125.11	114.35
2	A	1001	CIT	O6-C6-O5	3.21	134.12	123.86
2	A	1001	CIT	C3-C2-C1	2.95	121.98	113.92
2	A	1001	CIT	O4-C5-O3	-2.85	116.00	123.33
2	A	1001	CIT	O1-C1-C2	-2.80	115.01	122.95
2	A	1001	CIT	C3-C4-C5	2.25	120.08	113.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	CIT	O7-C3-C6-O6
2	A	1001	CIT	C1-C2-C3-O7
2	A	1001	CIT	C1-C2-C3-C4
2	A	1001	CIT	C1-C2-C3-C6
2	A	1001	CIT	O7-C3-C6-O5
2	A	1001	CIT	C2-C3-C6-O6
2	A	1001	CIT	C4-C3-C6-O5
2	A	1001	CIT	C4-C3-C6-O6
2	A	1001	CIT	C2-C3-C6-O5
2	A	1001	CIT	O1-C1-C2-C3
2	A	1001	CIT	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	CIT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	533/541 (98%)	0.31	35 (6%) 24 24	16, 36, 71, 81	0
1	B	514/541 (95%)	0.60	97 (18%) 3 2	17, 34, 112, 123	0
All	All	1047/1082 (96%)	0.45	132 (12%) 8 7	16, 35, 107, 123	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	THR	9.2
1	B	501	GLY	7.5
1	A	330	SER	6.3
1	B	470	HIS	6.0
1	B	490	PRO	5.8
1	B	500	ALA	5.4
1	B	530	LEU	5.2
1	A	540	GLY	5.1
1	B	497	LEU	5.1
1	B	539	GLY	5.0
1	B	325	GLY	5.0
1	B	498	LEU	4.9
1	B	528	ARG	4.9
1	B	444	TRP	4.9
1	B	463	ALA	4.8
1	B	526	LEU	4.8
1	B	493	LEU	4.7
1	B	187	THR	4.7
1	B	478	LEU	4.7
1	A	8	ALA	4.5
1	B	510	ALA	4.5
1	B	487	LYS	4.5
1	A	234	TRP	4.5
1	B	464	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	480	VAL	4.4
1	B	460	VAL	4.4
1	B	517	ILE	4.3
1	B	511	TYR	4.3
1	B	520	THR	4.3
1	B	496	HIS	4.2
1	A	328	GLU	4.2
1	B	538	TYR	4.2
1	B	371	GLU	4.1
1	B	442	GLY	4.1
1	B	441	GLY	4.0
1	B	445	ILE	4.0
1	B	302	GLY	4.0
1	B	532	GLU	4.0
1	B	512	VAL	4.0
1	B	509	ASP	3.9
1	A	187	THR	3.9
1	A	405	ARG	3.9
1	B	479	ALA	3.9
1	A	331	PRO	3.8
1	B	529	ALA	3.7
1	B	315	ARG	3.7
1	B	513	PHE	3.6
1	B	468	ILE	3.6
1	A	327	THR	3.6
1	B	466	VAL	3.6
1	A	302	GLY	3.5
1	A	326	LEU	3.5
1	B	537	TYR	3.5
1	B	453	ALA	3.5
1	A	188	THR	3.4
1	B	516	GLU	3.4
1	B	536	ASN	3.4
1	B	518	PRO	3.3
1	B	432	ASP	3.3
1	B	461	LYS	3.2
1	B	534	TYR	3.2
1	B	482	VAL	3.2
1	B	535	LYS	3.2
1	B	448	VAL	3.2
1	B	525	PHE	3.1
1	B	469	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	481	VAL	3.1
1	B	477	PRO	3.0
1	B	454	LEU	3.0
1	B	439	LYS	3.0
1	B	494	ASN	3.0
1	A	402	GLU	2.9
1	A	503	ALA	2.9
1	B	531	ARG	2.9
1	A	403	ALA	2.9
1	B	434	LEU	2.9
1	A	371	GLU	2.9
1	A	401	GLU	2.9
1	B	331	PRO	2.8
1	B	467	ALA	2.8
1	B	450	LEU	2.7
1	A	473	TRP	2.7
1	A	293	LYS	2.7
1	A	479	ALA	2.7
1	B	304	ALA	2.7
1	B	514	ALA	2.7
1	B	186	GLY	2.7
1	A	231	VAL	2.7
1	B	489	THR	2.7
1	B	459	LYS	2.7
1	A	404	THR	2.7
1	B	465	VAL	2.6
1	B	486	GLU	2.6
1	B	447	SER	2.6
1	B	533	GLN	2.6
1	B	527	LYS	2.6
1	A	189	GLY	2.6
1	B	458	PRO	2.5
1	B	499	LYS	2.5
1	B	329	THR	2.5
1	B	519	ARG	2.4
1	B	455	MET	2.4
1	B	515	GLU	2.3
1	B	234	TRP	2.3
1	A	406	SER	2.3
1	B	438	ILE	2.3
1	A	490	PRO	2.3
1	B	433	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	517	ILE	2.3
1	B	476	ARG	2.3
1	B	421	VAL	2.2
1	A	533	GLN	2.2
1	B	327	THR	2.2
1	B	437	LEU	2.2
1	A	291	ARG	2.2
1	B	488	PRO	2.2
1	B	348	GLU	2.2
1	B	347	GLU	2.1
1	B	402	GLU	2.1
1	A	152	LYS	2.1
1	A	474	GLN	2.1
1	B	452	ASN	2.1
1	A	498	LEU	2.1
1	B	7	ASN	2.1
1	B	188	THR	2.1
1	A	433	ARG	2.1
1	B	443	GLU	2.1
1	A	305	ALA	2.1
1	B	303	SER	2.1
1	A	487	LYS	2.0
1	B	326	LEU	2.0
1	B	446	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	A	1001	13/13	0.76	0.18	81,84,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.